Amendments to the Abstract

Please replace the abstract on page 32 with the following amended abstract.

A method for designing a metal ion for use in a ~~MD~~ molecular dynamics simulation can include the steps of building a metal ion molecule having a center atom and a dummy atom, assigning a van der Waals radius to the center atom, and assigning a charge to the dummy atom. A metal ion molecule may have~~.~~ ~~T~~[t]he center atom covalently linked to one or more dummy atoms resulting in the metal ion molecule having a polyhedron geometry. New force field parameters may be used in methods for designing metal ions for use in ~~MD~~ molecular dynamics simulations.